Chlorothalonil
1897-45-6 | DTXSID0020319

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 103

Global applicability domain: Inside

Local applicability domain index: 3.36e-01

Confidence level: 6.72e-01

Nearest Neighbors from the Training Set

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Kepone
Measured: 1550
Predicted: 1380

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1-Chloro-4-nitrobenzene
Measured: 20.0
Predicted: 12.2

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2,3-Dichloronitrobenzene
Measured: 145
Predicted: 70.0

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Trichloroethylene
Measured: 15.8
Predicted: 15.2

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2,4-Dichloronitrobenzene
Measured: 117
Predicted: 55.3